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**DIELECTRIC AND PLASMONIC PARTICLES ENABLING NANOSCALE
ENERGY ENGINEERING**

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Final Report

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This project focuses on manipulating the physics of dielectric and plasmonic nanostructures for transformative near and far fields applications. We mainly investigate 1) dielectric patterned crystals with optimized periodicities to engineer directive radiation emission, 2) plasmonic nanoparticles (and core-shell) for light concentration in near and far fields, 3) large array of plasmonic nanoparticles for energy engineering in layered substrates (solar cell application), and 4) modeling finite and non-periodic array of plasmonic dipole nanoantennas. The emphasis is on modeling and physical understanding. Here we present a summary where all details can be found in our publications (reference section). Students have been involved and trained in depth in such emerging areas.

1. Dielectric Patterned QCL Emission

We design a crystal, of dielectric rods, of different periodicities in transverse and propagating directions such that a spherical wave can be engineered to a plane wave. Namely a defect is created and a point source is transformed to a plane wave at the band-edge frequency. The dispersion diagram is tailored and optimized successfully. We then integrate the system with a Quantum Cascade Laser (QCL) device to engineer its beam and provide a directive emission. Figs. 1-4 show some of the key results. Full details can be found in [1]. This is an extremely important topic in the area of QCL systems and the idea can even be extended to other areas when one is interested to shape the wavefront with only dielectric elements. The system can also be hybridized with molecules and quantum dots (QDs).

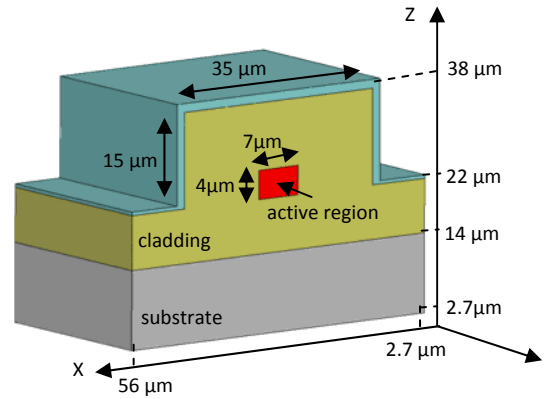


Fig. 1. The geometry of the QCL source. Active region is surrounded by cladding medium and generates an almost TEM wave.

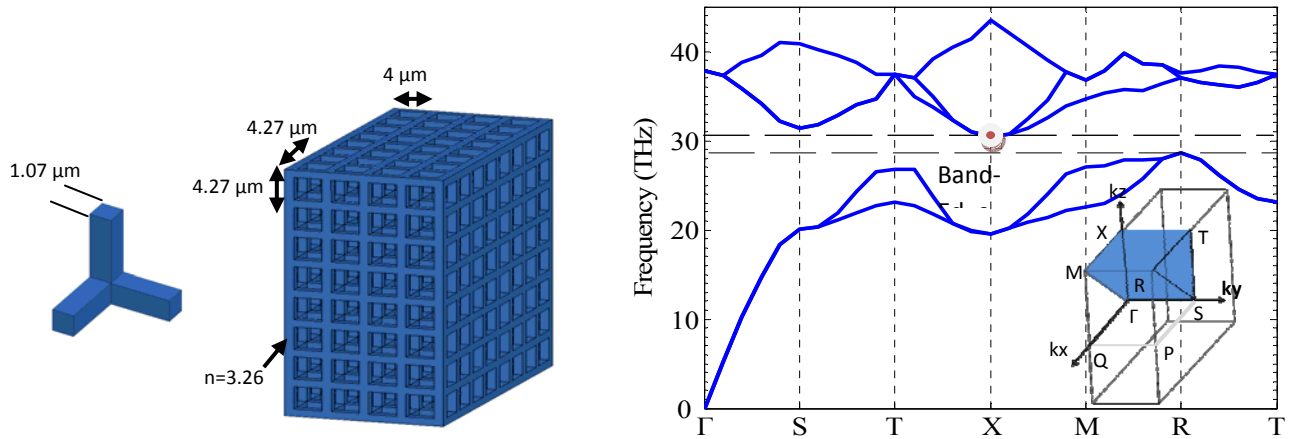


Fig. 2: (a) 3D PC metamaterial pattern with different periodicities in transverse and vertical directions, and (b) its dispersion diagram. The band-edge is clearly demonstrated.

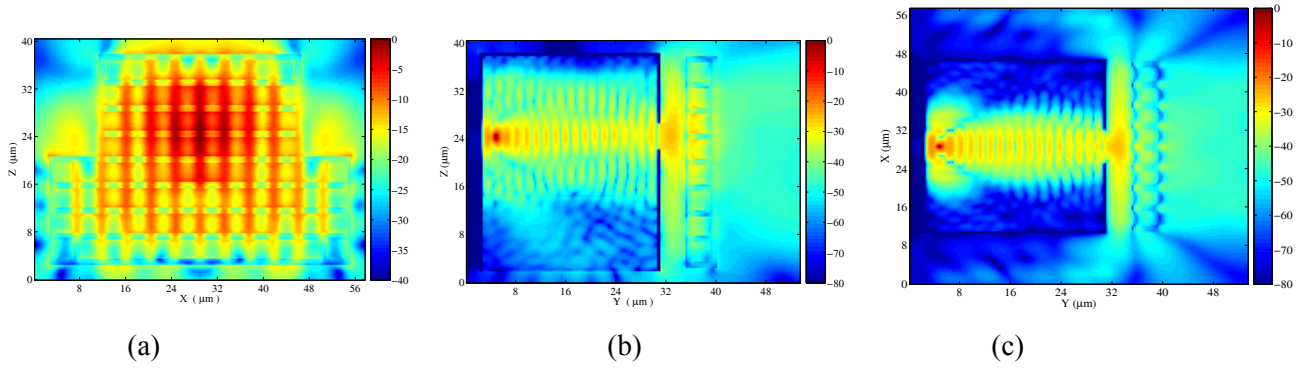


Fig. 3: Near-field distributions of the QCL integrated with dielectric nanoantenna on (a) the facet (x - z plane), (b) vertical plane (y - z plane), and (c) horizontal plane (x - y plane). As observed the fields are collimated away from the device.

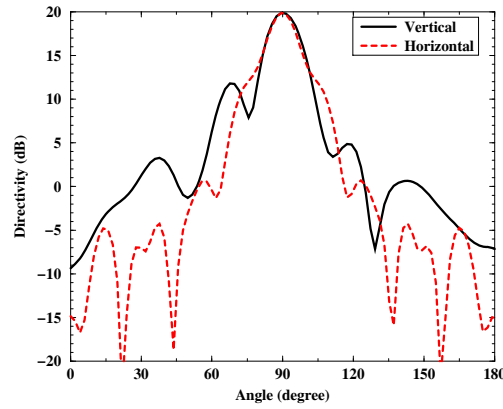
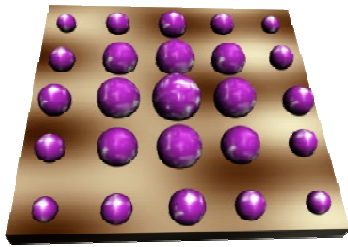


Fig. 4: Radiation performance of QCL nanoantenna demonstrating directive emission (20 dB) with narrow beamwidths of 14° and 12° in vertical and horizontal planes. The beam is tilted down by 5° in vertical plane due to the geometry asymmetry in this direction. Radiation patterns are plotted in pattern coordinate system.

2. Plasmonic Particles for Near and Far Fields Engineering

Plasmonics can provide strong near-fields in subwavelength scale. Engineering patterns of elements can significantly offer transformative physics in both near and far fields. We have investigated both areas in great depth [2-4]. Figs 5 and 6 show design of array of core-shells where they can engineer the near fields and achieve a required profile. We start with a desired function and produce required elements for the functionality of interest [2]. Dipole mode analysis and proper dyadic Green's functions in comprehensive way are developed for large array simulation, fast and accurate. A nonlinear optimization approach is used for obtaining the required design. Full mathematical equations can be found in [2].



$$p_x^n = \alpha_n \left(\sum_{m=1, m \neq n}^N (G_{xx, z=0}^{nm} p_x^m + G_{xy, z=0}^{nm} p_y^m) + G_{xy, z=0}^{n0} p_{source} \right)$$

$$p_y^n = \alpha_n \left(\sum_{m=1, m \neq n}^N (G_{yx, z=0}^{nm} p_x^m + G_{yy, z=0}^{nm} p_y^m) + G_{yy, z=0}^{n0} p_{source} \right)$$

$$\bar{\mathbf{G}}(\mathbf{r}, \mathbf{r}') = \frac{1}{4\pi\epsilon_0} \frac{e^{-jk_0 R}}{R^3} \left\{ \left[(k_0 R)^2 - jk_0 R - 1 \right] \bar{\mathbf{I}} - \left[(k_0 R)^2 - j3k_0 R - 3 \right] \frac{\mathbf{R}\mathbf{R}}{R^2} \right\}$$

Fig. 5: Plasmonic elements for near-field engineering and some of the required equations.

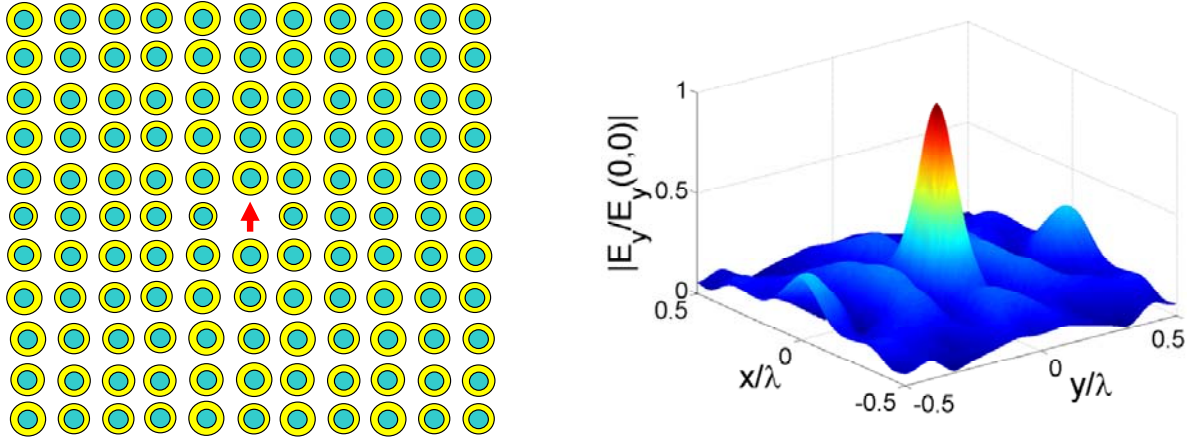


Fig. 6: 11x11 array of core-shells, modeled and optimized to concentrate the beam in subwavelength scale.

Similar concept can be implemented for far-field engineering. We implement for the first time the concept of reflectarray in optics. Basically the elements are engineered to locally control the phase of scattered light and scan the beam in a direction of interest. This is of extreme importance for successful wave engineering, with subwavelength elements, in optics. Full details can be found in [3]. Figs 7 and 8 also show the design procedure.

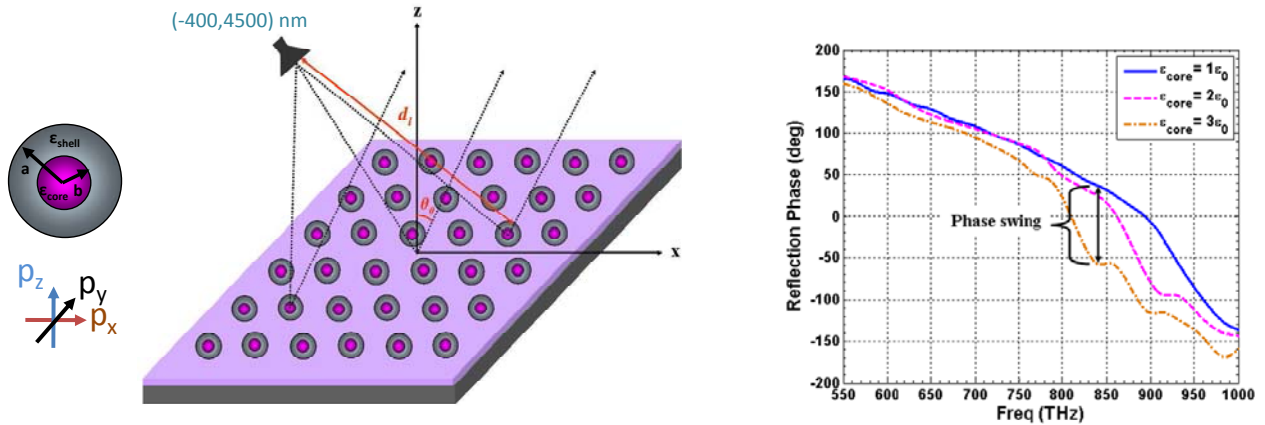


Fig. 7: Non-uniform array of core-shell plasmonic particles and their design phase curve. The curve can successfully be used to obtain required core-shell design.

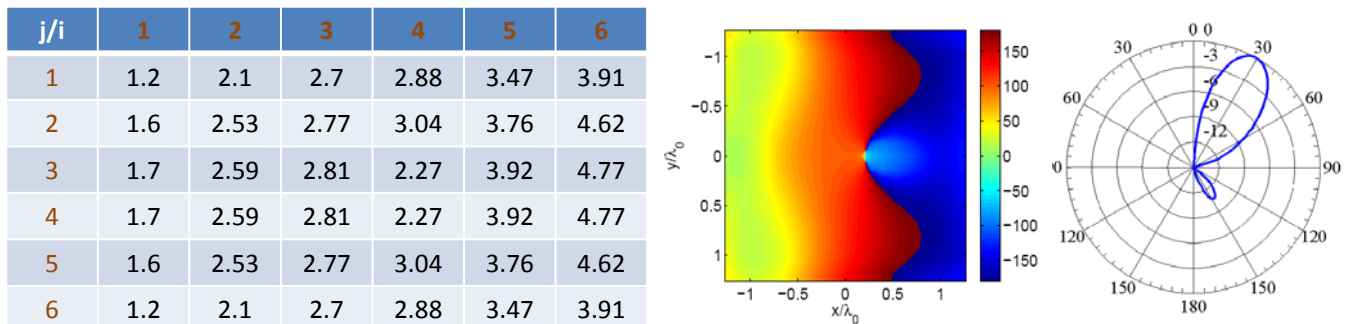


Fig. 8: Characteristics of the array depicted in Fig. 7, and the field performance. The beam is successfully scanned (directed and tilted) to desired direction.

While in above gold material is used, one can consider integration of other materials like ITO, AZO, GZO where they can have functionality (negative permittivity) in other optical bands of interest. A comprehensive investigation (using dipolar modes) is performed to obtain the dispersion diagram and achieve unique physics, such as double negative and backward wave behaviors. This is of remarkable importance to metamaterial community (when they can decide to choose the right material for an application in hand). Full details can be found in [4]. Below shows some of the examples.

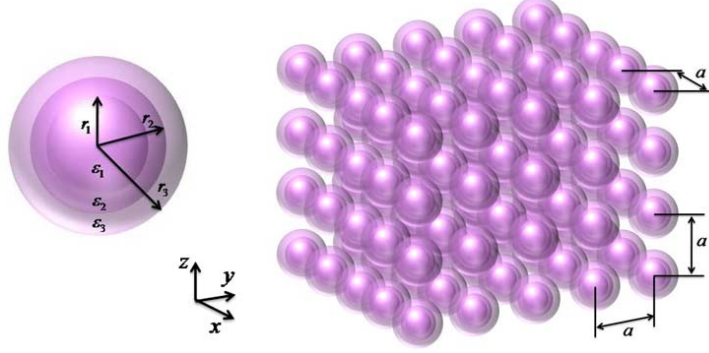


Fig. 9: Configuration of an array of multimaterial multilayer spheres.

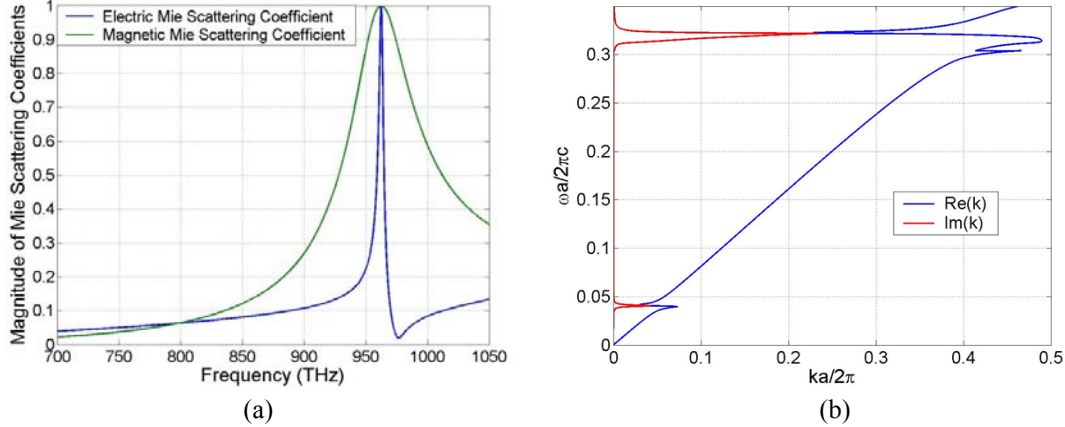


Fig.10: (a) Normalized electric and magnetic Mie scattering coefficients of a single two-layer sphere with silver shell, and (b) real and imaginary parts of dispersion diagram for the element used in array structure of Figure 1 with unit cell $a=100nm$ ($r_1=33.77nm$ and $r_2=35nm$).

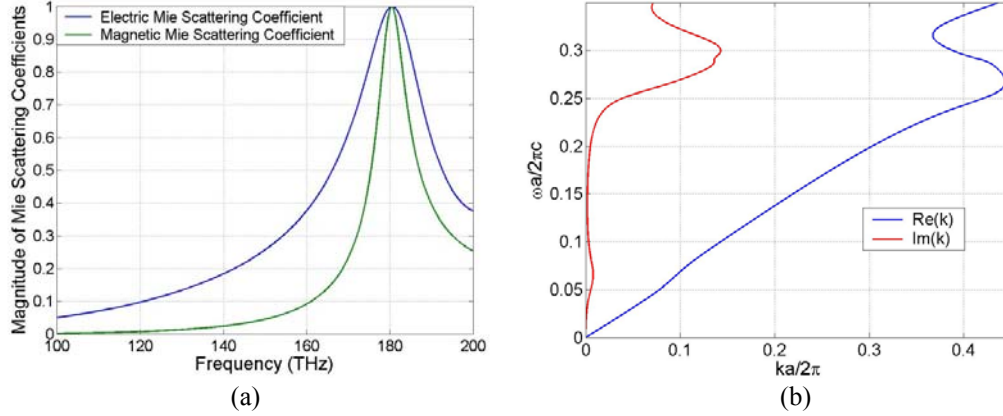


Fig. 11: (a) Normalized electric and magnetic Mie scattering coefficients of a single two-layer sphere with AZO shell, and (b) real and imaginary parts of dispersion diagram for the element used in the array structure with unit cell $a=500\text{nm}$ ($r_1=181.5\text{nm}$ and $r_2=212\text{nm}$).

Table 1. Designed two and three layer spheres parameters – A comparison study.

Shell	r_1 [nm]	r_2 [nm]	a [nm]	ω_r [THz]	$Max[Im(ka)]$
Gold	20.7	22	75	1575	1.32
Silver	33.77	35	100	960	1.445
ITO	166.6	201	450	196.88	0.94
AZO	181.5	212	500	180.4	0.85
GZO	160	194	450	205.2	0.9
3-Layer 2 nd layer: Gold $r_3=139.9\text{nm}$	25	29	120	898.1	2.07

3. Plasmonic Elements on Layered Substrate

As soon as one considers plasmonic elements to be on a layered substrate the whole formulation will be affected in great depth. The problem is that the free space Green's functions must be changed to those for layered structures and Sommerfeld integrals must come into the picture, which they have very slow convergence. We need to add to this that for many applications a large array of plasmonic particles (and not necessarily periodic) is sitting on the substrate making the computation very challenging. This is a very complex problem, but of significant interest to energy and solar cell community. We have proposed for the first time a very novel and fast method to solve such structures. We model the effect of layered substrate with complex image sources. We have to deform the contour path for Sommerfeld integrals smartly to manage the problem, successfully. We use dipolar mode analysis for large array of spheres and consider polarization in all three directions. A full wave study is performed and the details can be found in our work published in [5]. This is an entirely unique modeling approach for solving large array of plasmonic nanoparticles on layered substrates, tailoring novel physics and applications. Figs 12-14 show some of the results.

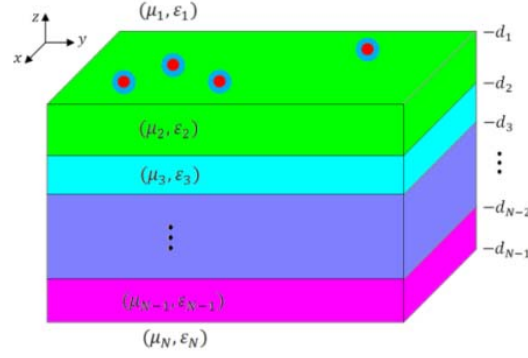


Fig. 12. Array of plasmonic nanoparticles on a planarly multilayered medium.

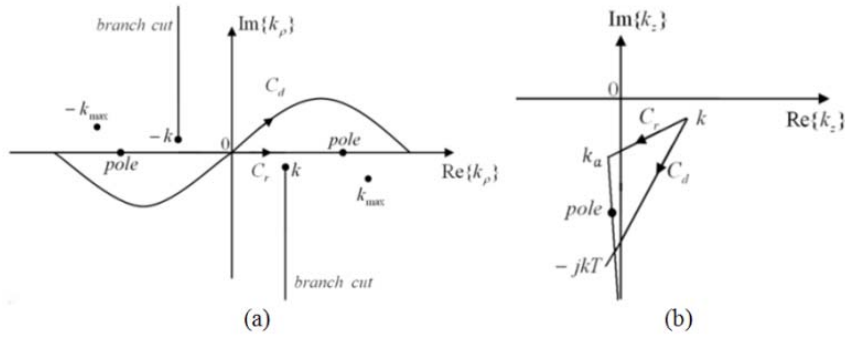


Fig. 13. Integration contours C_r and C_d (a) in complex k_ρ -plane and (b) in complex k_z -plane. Deformation is performed for proper integration.

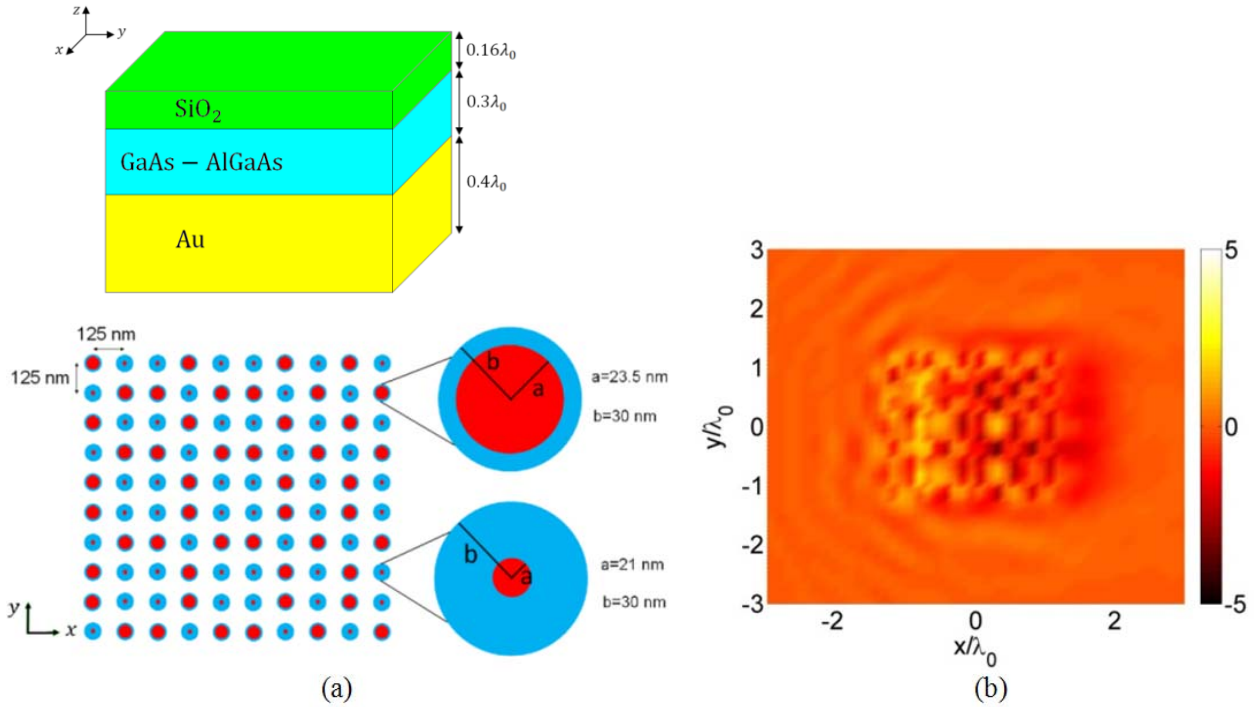


Fig. 14. (a) An aperiodic array of 100 plasmonic nanoparticles sitting on SiO₂-GaAs-AlGaAs-Au substrate (b) $|E|^2$ (dB) at the middle of the GaAs-AlGaAs layer. Field enhancement is observed in compared to case with no array.

4. Finite and Non-Periodic Array of Dipole Nanoantennas

So far our focus has been on sphere (and multilayer shell) configurations. However, for many practical applications, other geometries can become of interest, like dipole nanorods. The main issue is one cannot use dipolar modes approach obtained using Mie series to solve the problem anymore. A new way of thinking must be implemented. Here we apply Characteristics Basis Functions Method (CBFM). Basically we start with a nanorod and excite it from different directions, then solve it with MoM obtaining the solution for each excitation. Not all solutions are independent. We will apply mathematical approach SVD to obtain the linear independent solutions. It turns out one can end up to only few basis functions representing the physics of the nanorod. Then for an array we replace each element with those few basis functions (and only few unknowns instead of the original problem which can include hundreds unknowns); and manage to solve a very large array of plasmonic nanorods and of random distribution in a successful way, very fast and accurate (orders of magnitude improvements in compared to traditional approaches). Full details can be found in [6-8]. Figs 15-20 shows some of the key results.

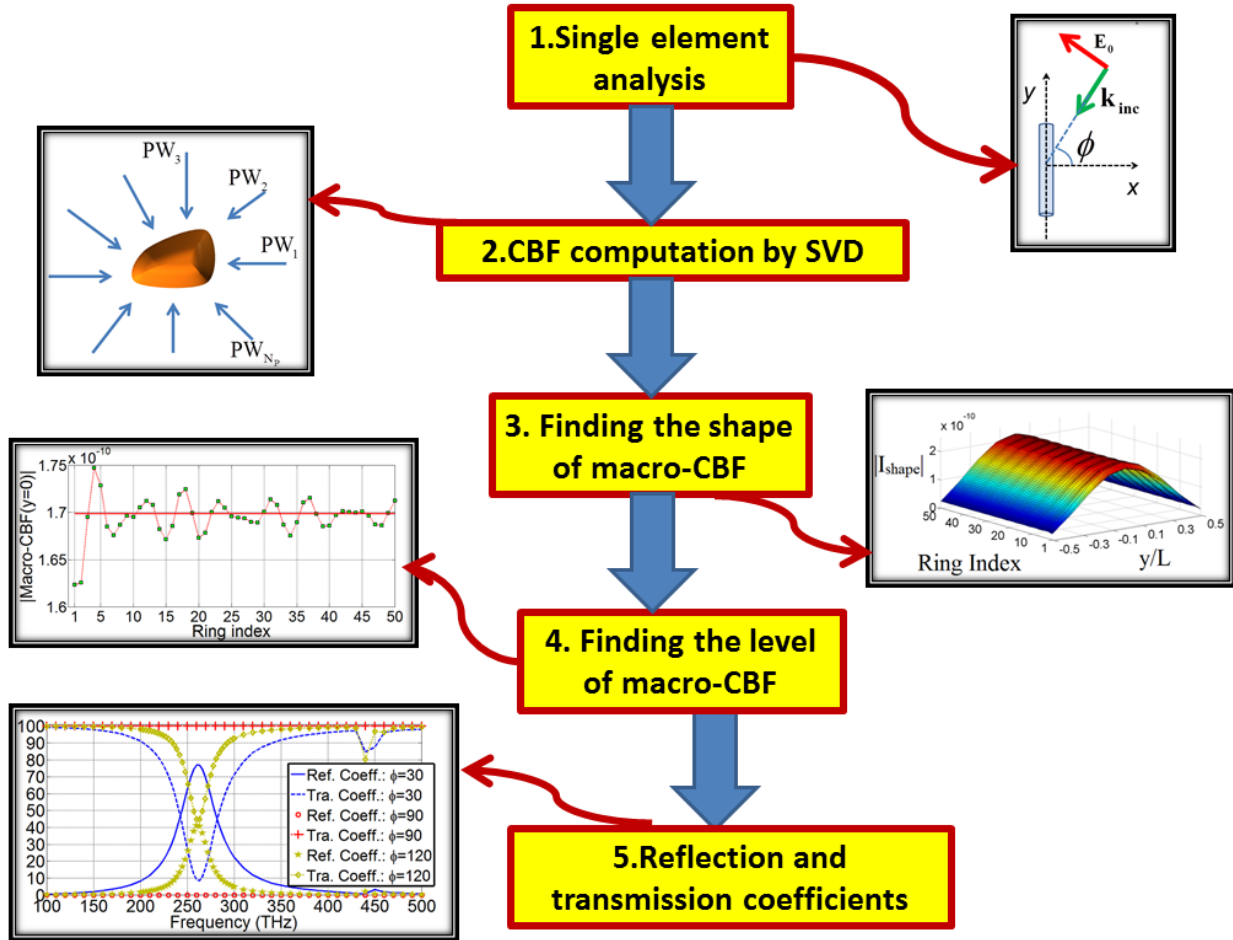


Fig. 15: Organizational flowchart of CBFM computational model.

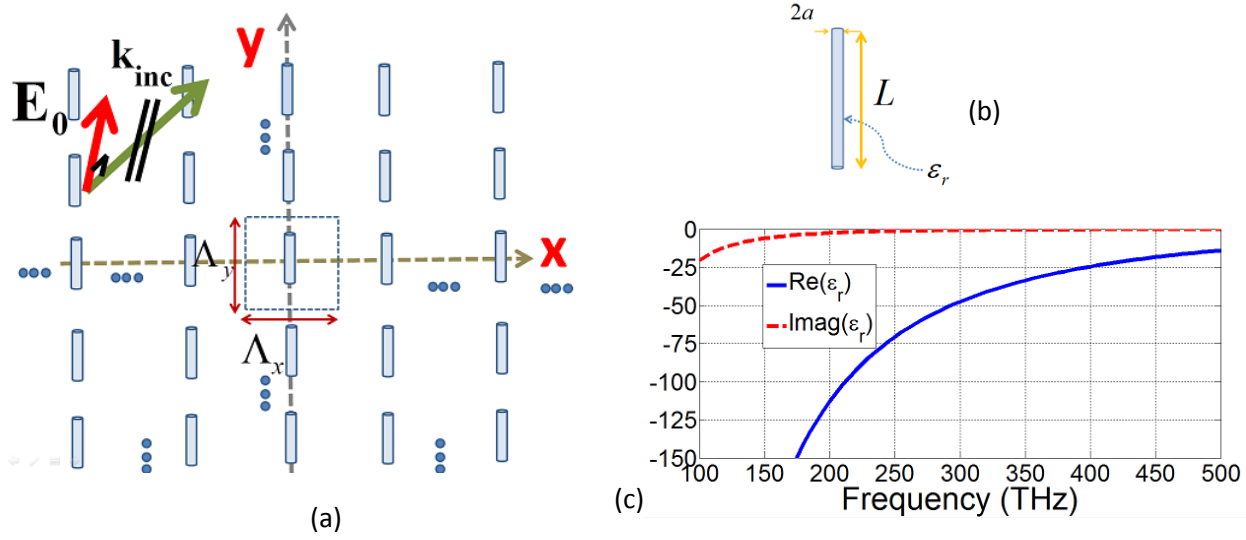


Fig. 16: (a) Two-Dimensional array of plasmonic nanorods illuminated by an oblique incident plane wave. The periods along x- and y-axis are Λ_x and Λ_y , (b) The plasmonic nanorod made of a Drude material as the unit-cell, (c) Real part and imaginary part of the permittivity of silver over a desired optical frequency range.

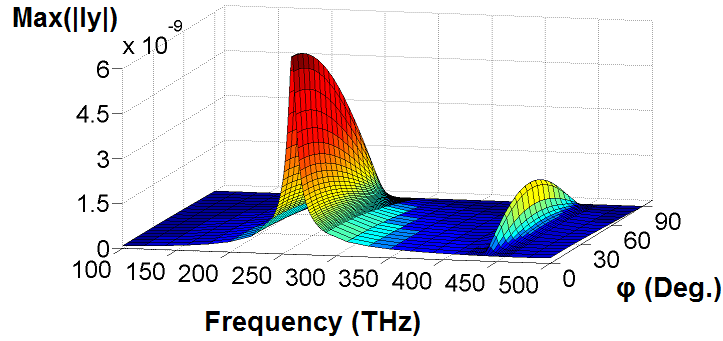


Fig. 17: Maximum of the magnitude of the longitudinal current versus the frequency and the azimuthal incident angle (ϕ).

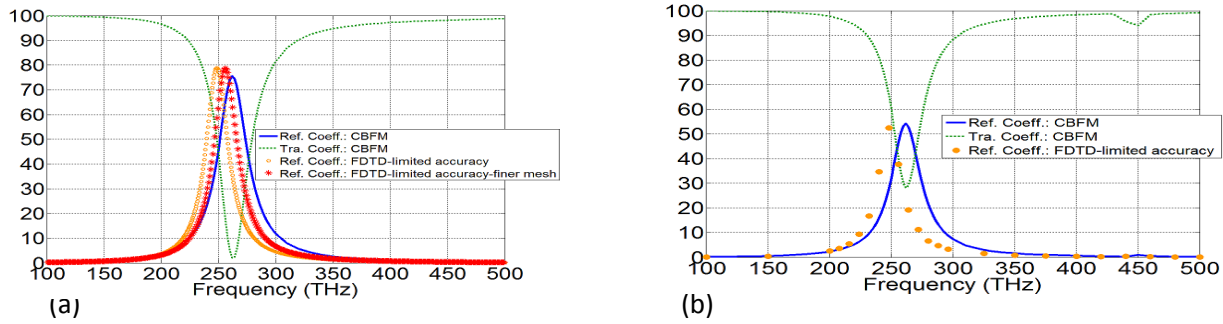


Fig. 18: Reflection and transmission coefficients (in percentage) for normal and oblique incidence cases compared with FDTD. The FDTD result is with limited accuracy due to the mesh-size. (a) Normal incidence, (b) Oblique incidence.

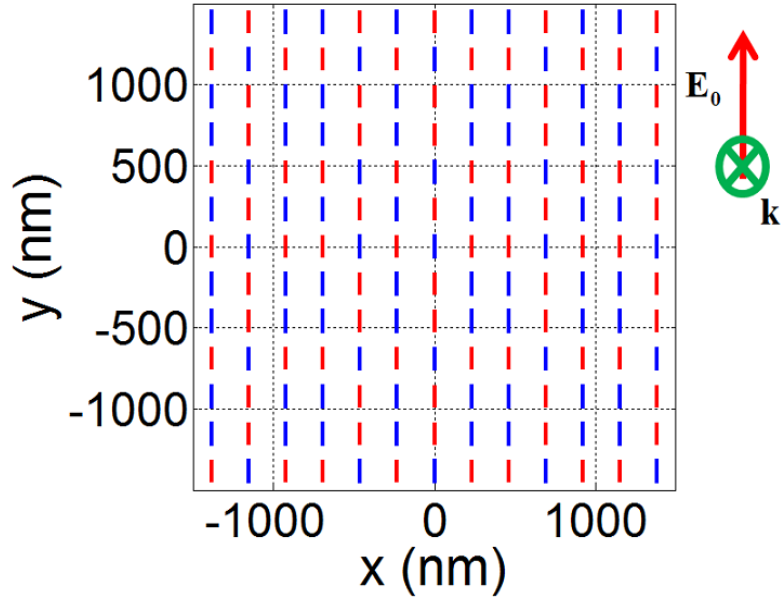


Fig. 19: Fibonacci quasi-lattice of order 6, 13×13 . The array comprises of two different plasmonic nanorods, blue nanorod with lower resonant and red with higher resonant frequencies.

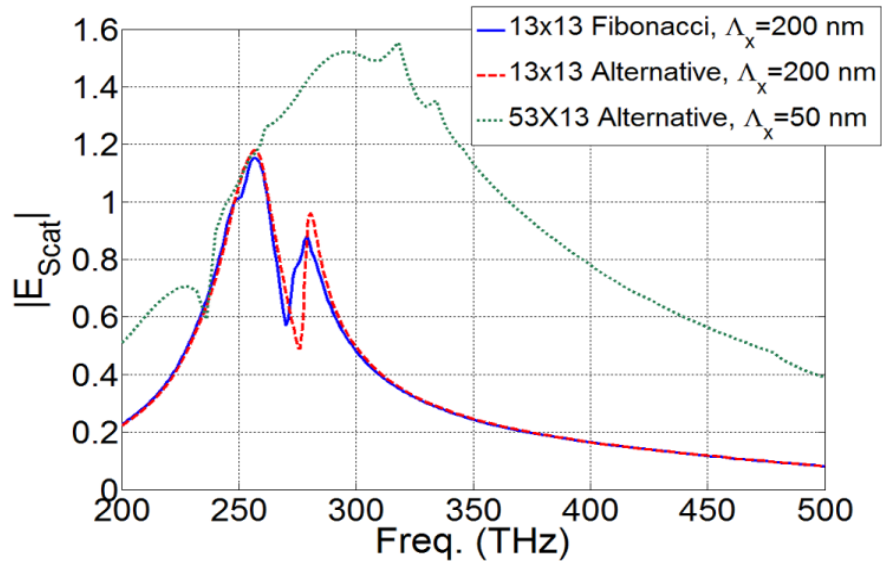


Fig. 20: The optical performance of the Fibonacci and alternative quasi-lattices of plasmonic nanorods. Bringing the elements closer to each other can merge the two resonances.

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